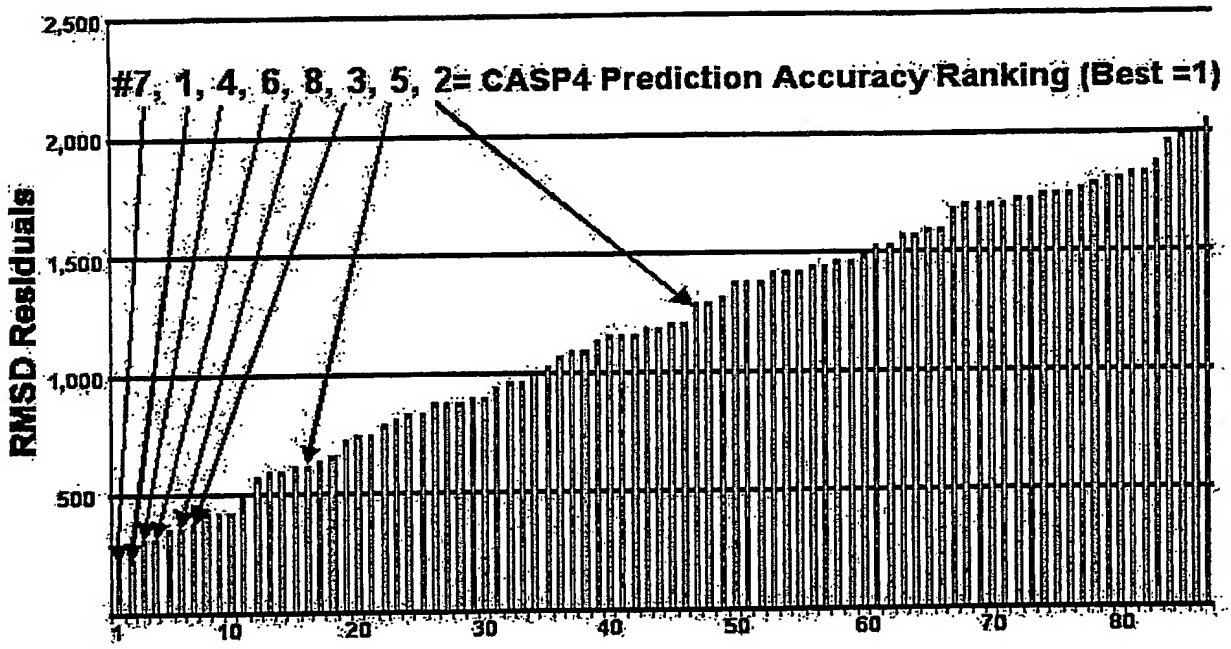

Figure 1

BEST AVAILABLE COPY

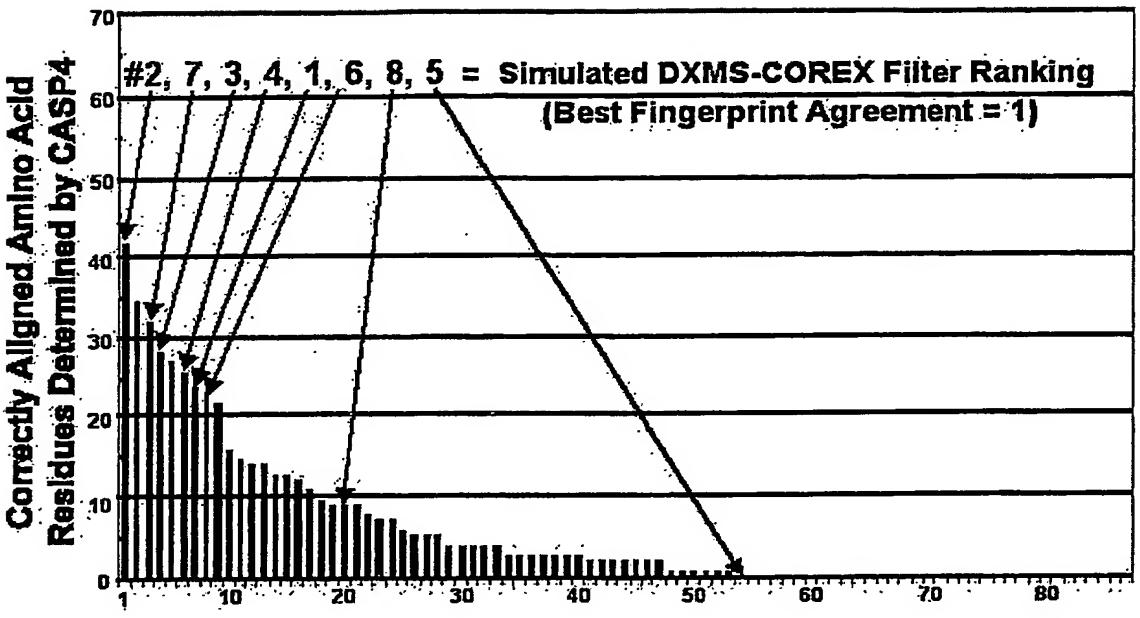
#2, 7, 3, 4, 1, 6, 8, 5 = Simulated DXMS-COREX Filter Ranking
(Best Fingerprint Agreement = 1)
Correctly Aligned Amino Acid Residues Determined by CASP4
70
60
50
40
30
20
10
0
1
10
20
30
40
50
60
70
80

Figure 2

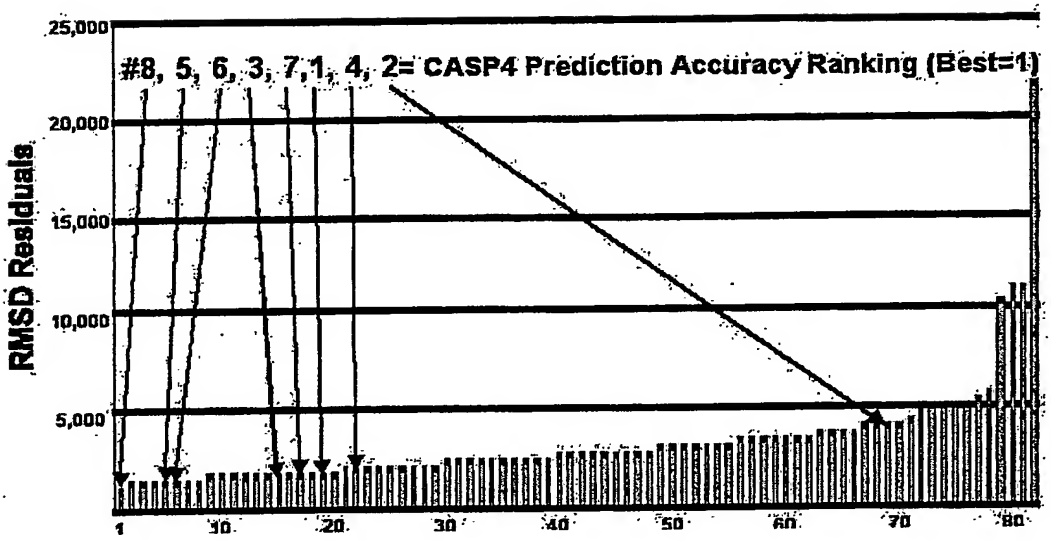
#8, 5, 6, 3, 7, 1, 4, 2= CASP4 Prediction Accuracy Ranking (Best=1)
RMSD Residuals
25,000
20,000
15,000
10,000
5,000
1
10
20
30
40
50
60
70
80

Figure 3

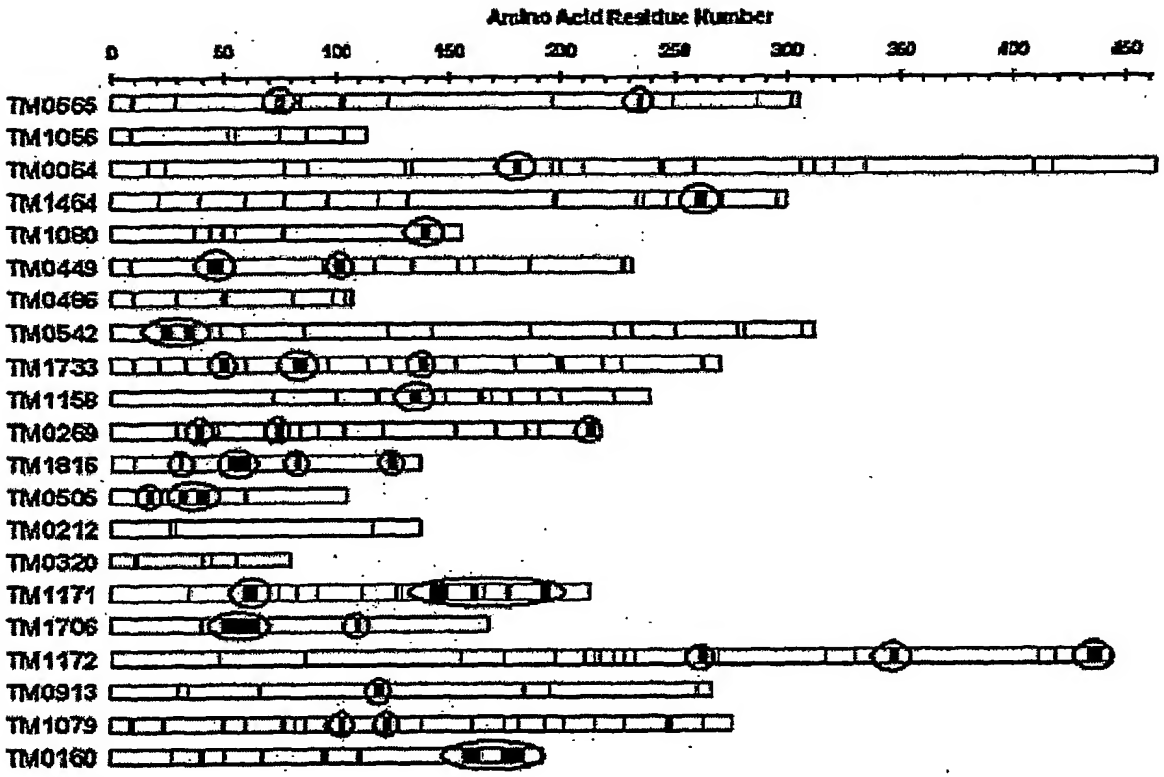
Amino Acid Residue Number
0
50
100
150
200
250
300
350
400
450
TM0565
TM1056
TM0064
TM1464
TM1080
TM0449
TM0496
TM0542
TM1733
TM1158
TM0269
TM1815
TM0505
TM0212
TM0320
TM1171
TM1706
TM1172
TM0913
TM1079
TM0160

Figure 4

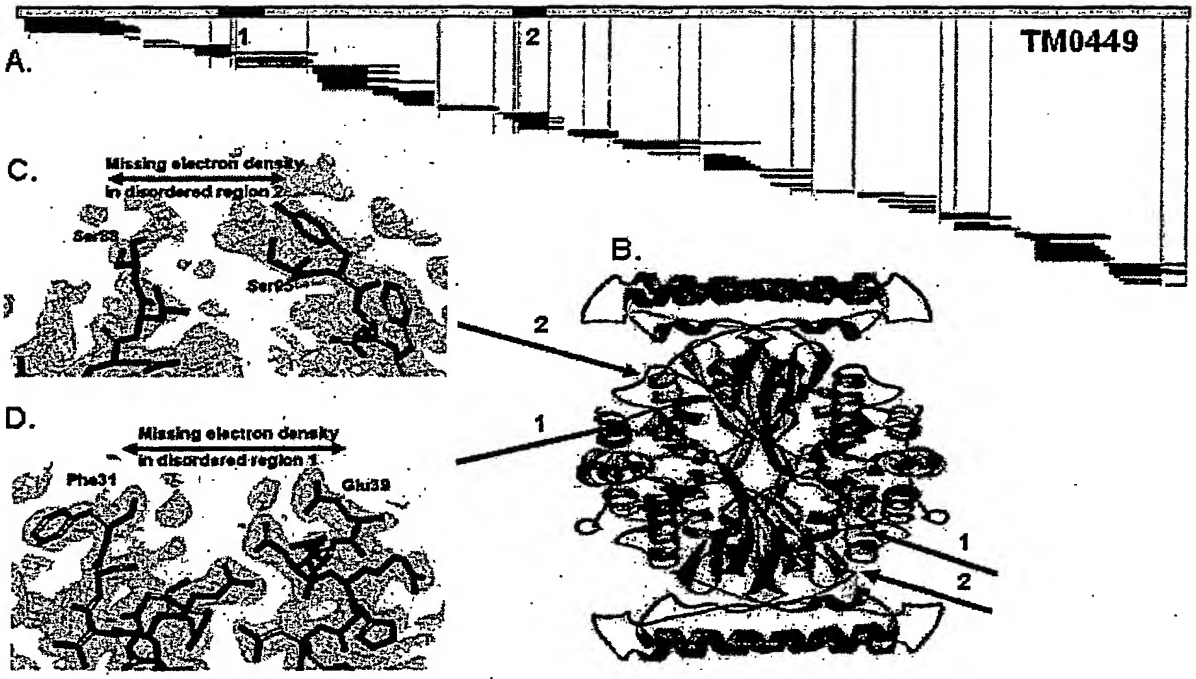
A.
1
2
TM0449
C.
Missing electron density
in disordered region 2
Ser28
Ser3
B.
2
1
D.
Missing electron density
in disordered region 1
Phe31
Glu39
1
2

Figure 5

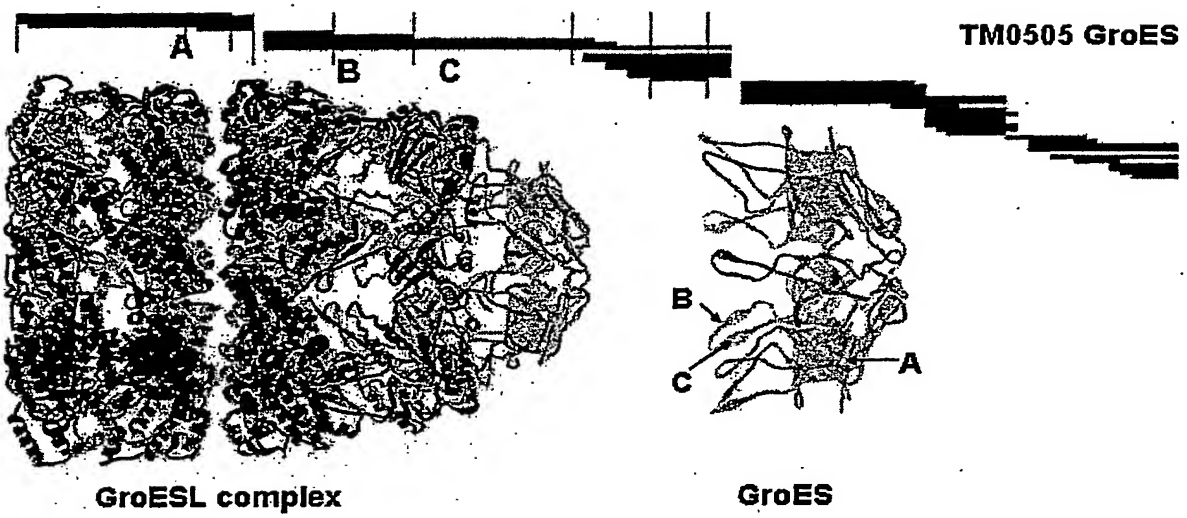

Figure 6

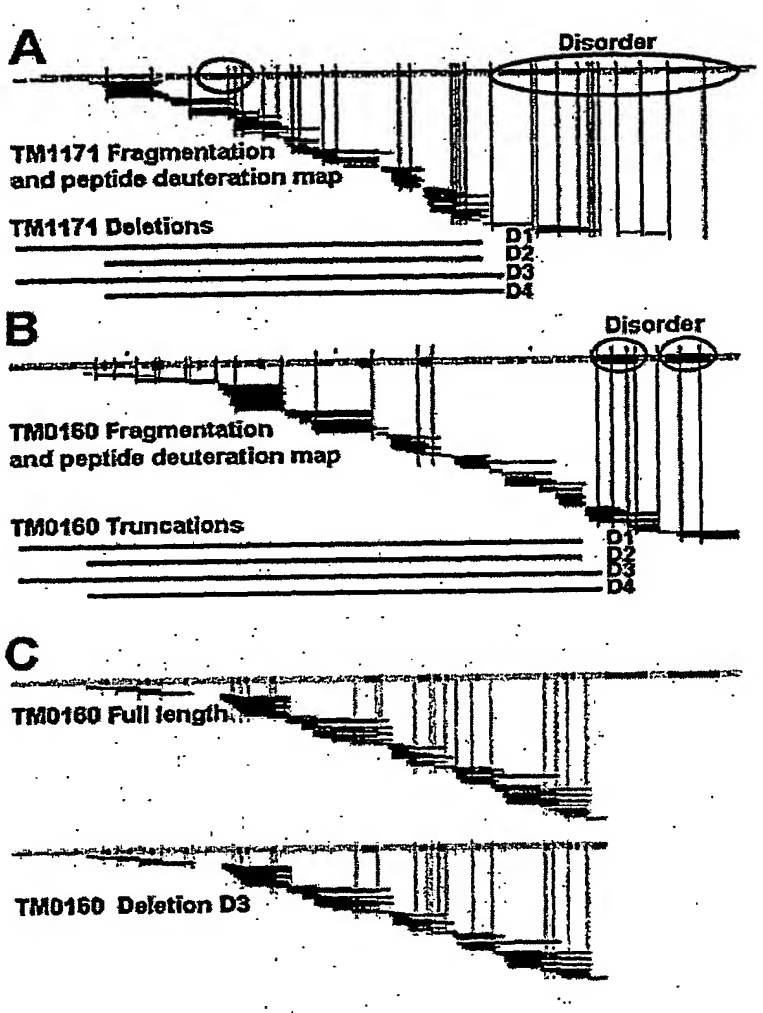
A
Disorder
TM1171 Fragmentation
and peptide deuteration map
TM1171 Deletions
D1
D2
D3
D4
B
Disorder
TM0160 Fragmentation
and peptide deuteration map
TM0160 Truncations
D1
D2
D3
D4
C
TM0160 Full length
TM0160 Deletion D3

Figure 7

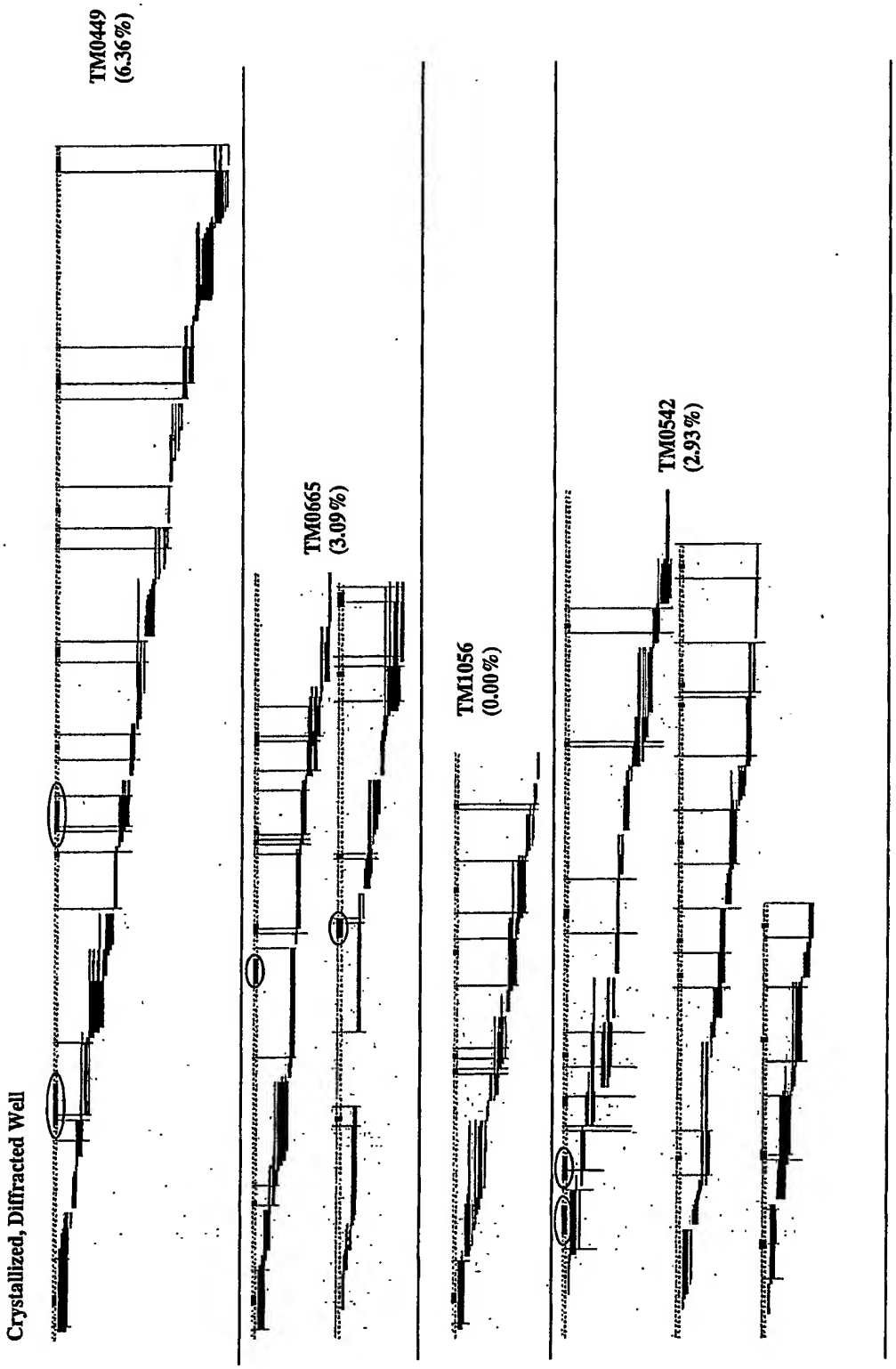
Crystallized, Diffracted Well
TM0449
(6.36%)
TM0665
(3.09%)
TM1056
(0.00%)
TM0542
(2.93%)

Figure 8A

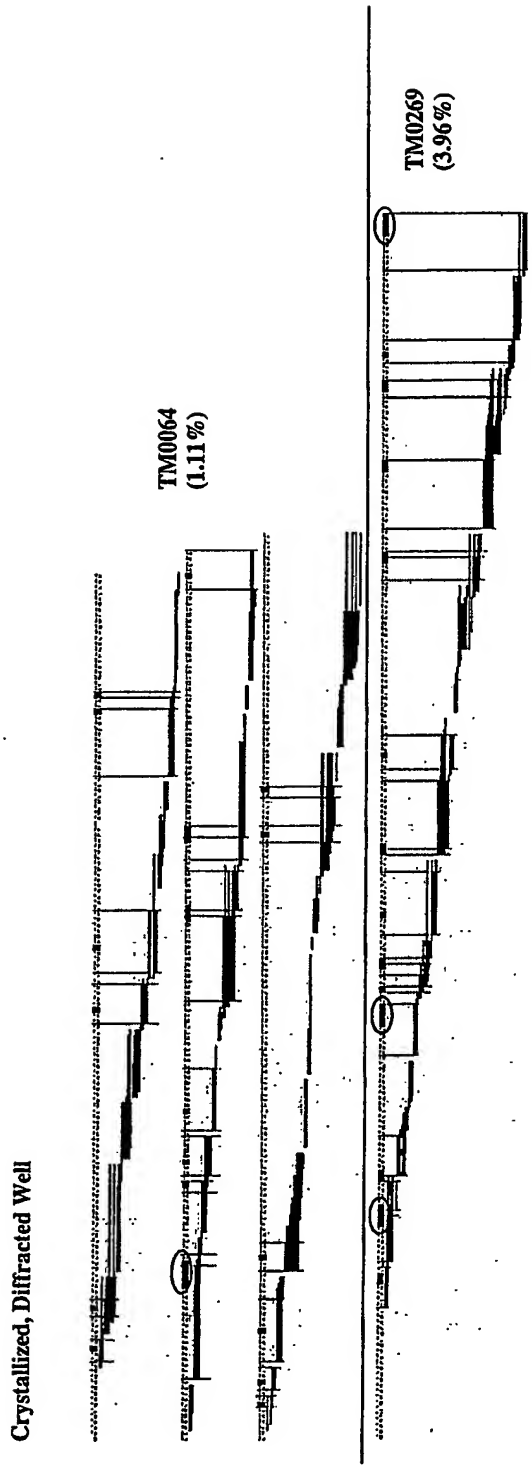

Figure 8B

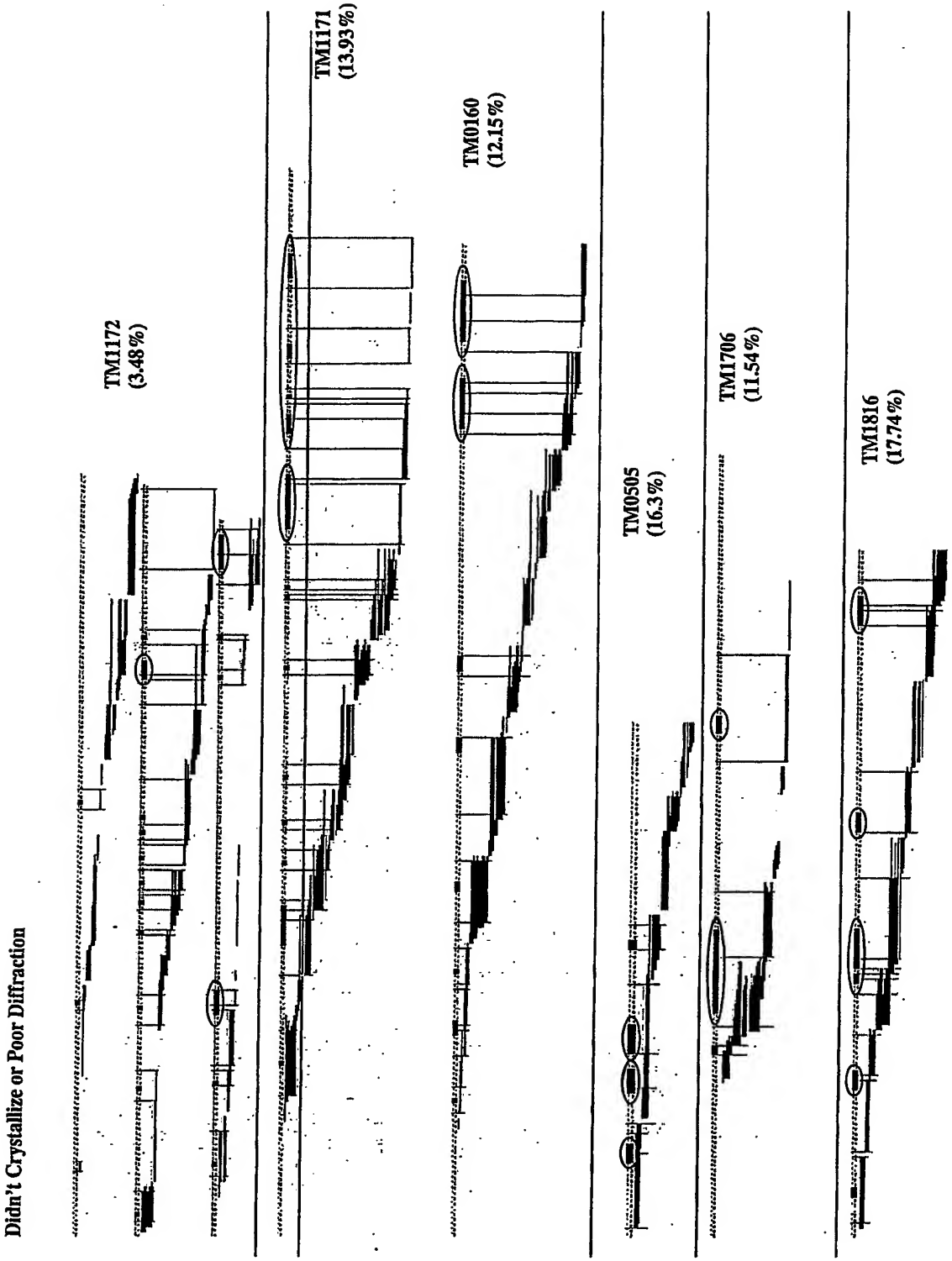
Didn't Crystallize or Poor Diffraction
TM1172
(3.48%)
TM1171
(13.93%)
TM0160
(12.15%)
TM0505
(16.3%)
TM1706
(11.54%)
TM1816
(17.74%)

Figure 8C

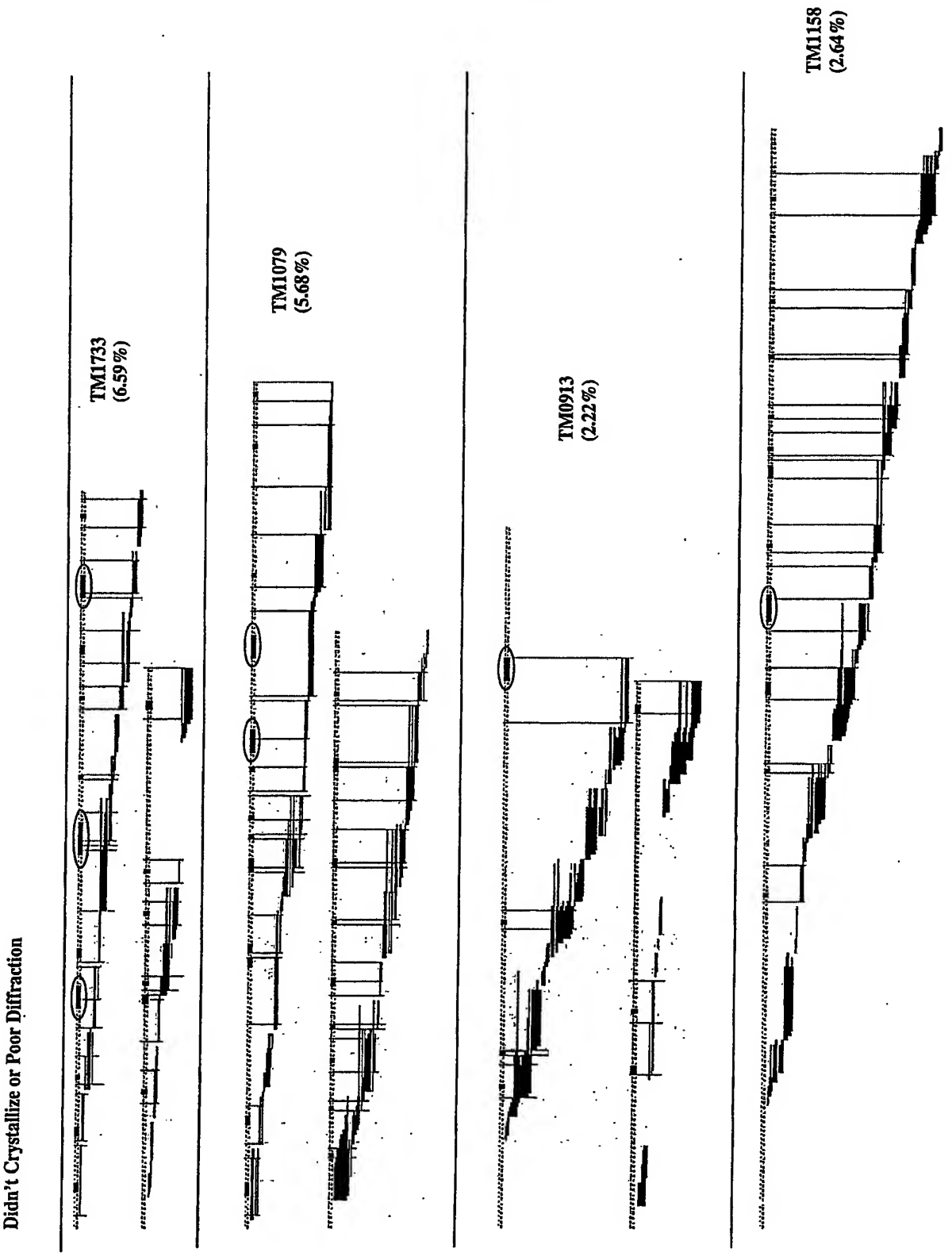
TM1733
(6.59%)
TM1079
(5.68%)
TM0913
(2.22%)
TM1158
(2.64%)
Didn't Crystallize or Poor Diffraction

Figure 8D

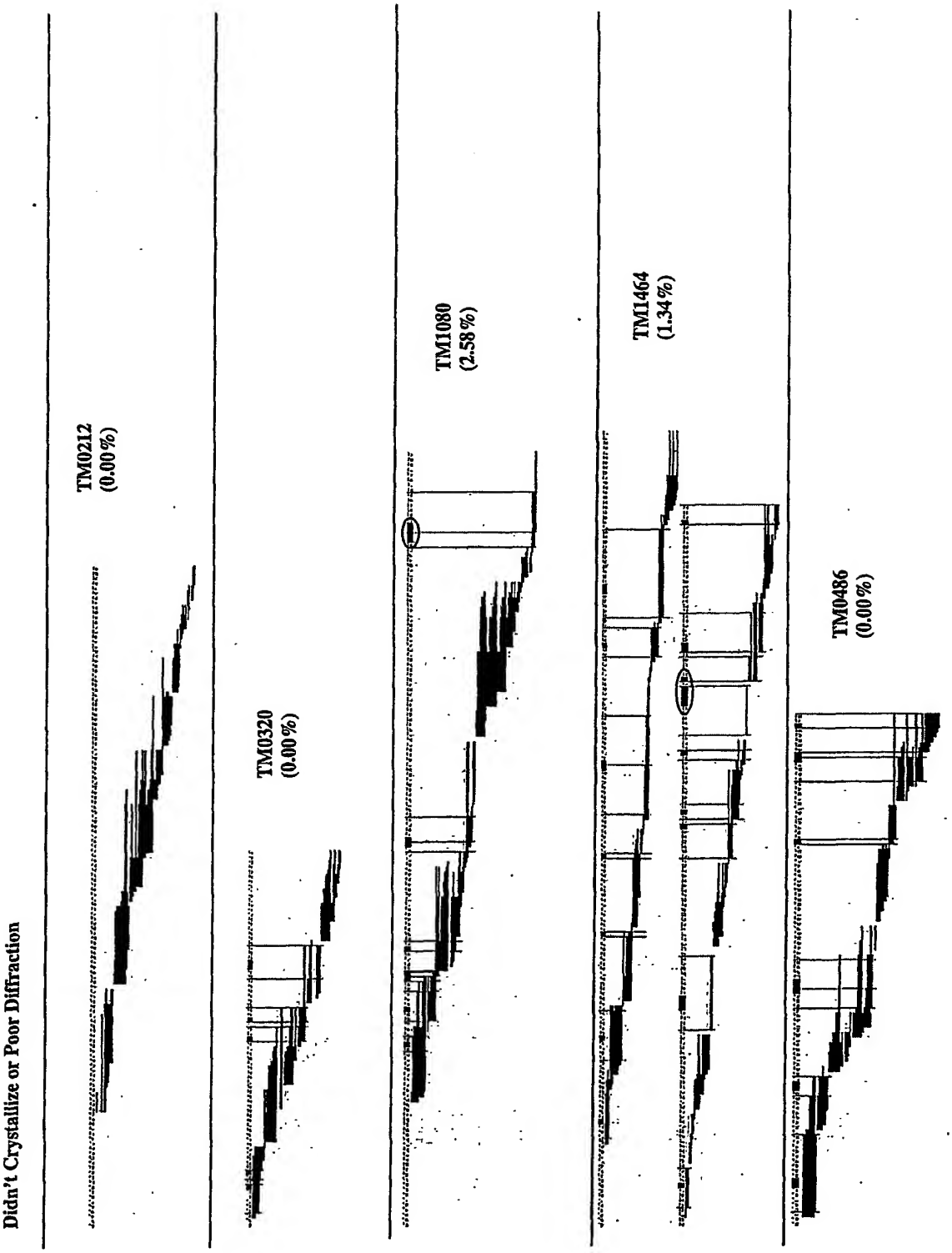
Didn't Crystallize or Poor Diffraction
TM0212
(0.00%)
TM0320
(0.00%)
TM1080
(2.58%)
TM1464
(1.34%)
TM0486
(0.00%)

Figure 8E

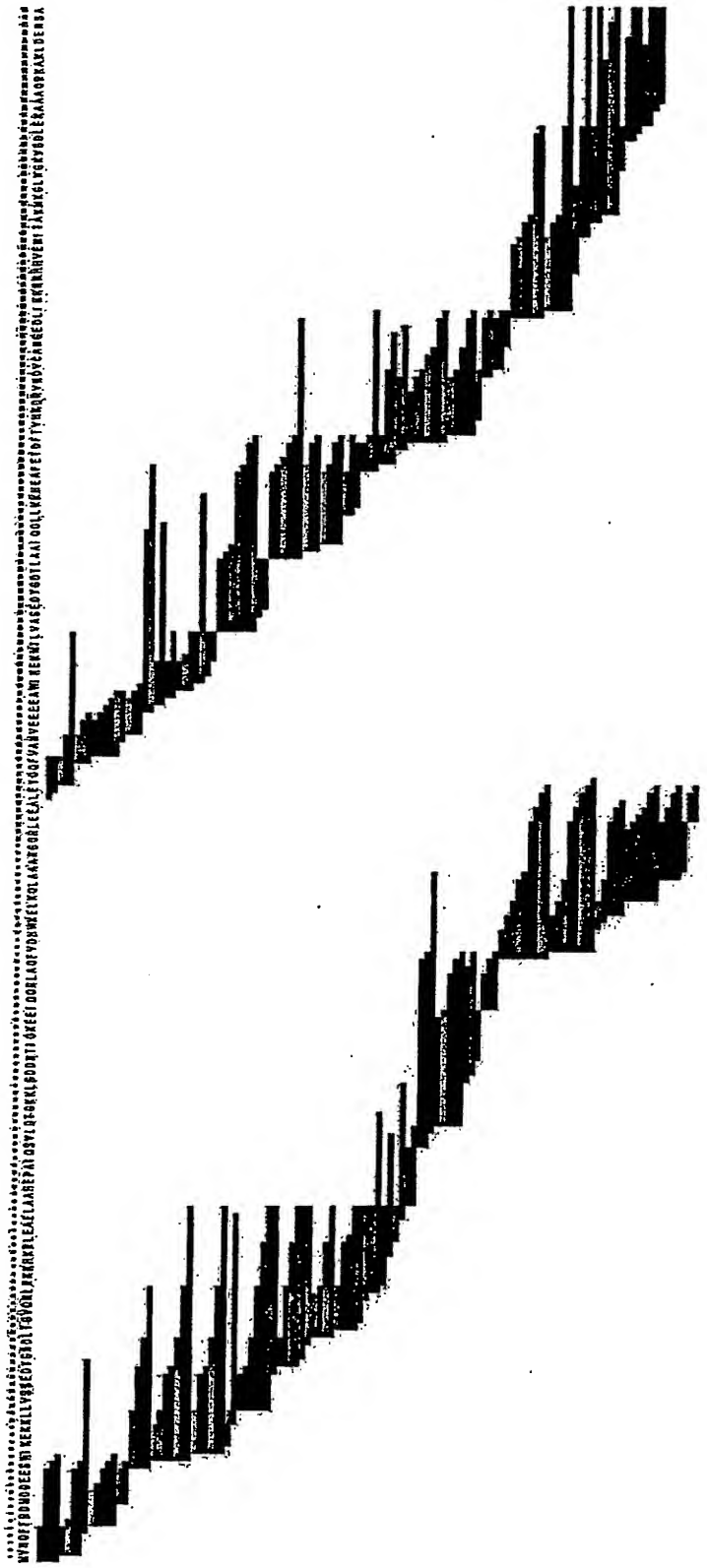

Figure 9

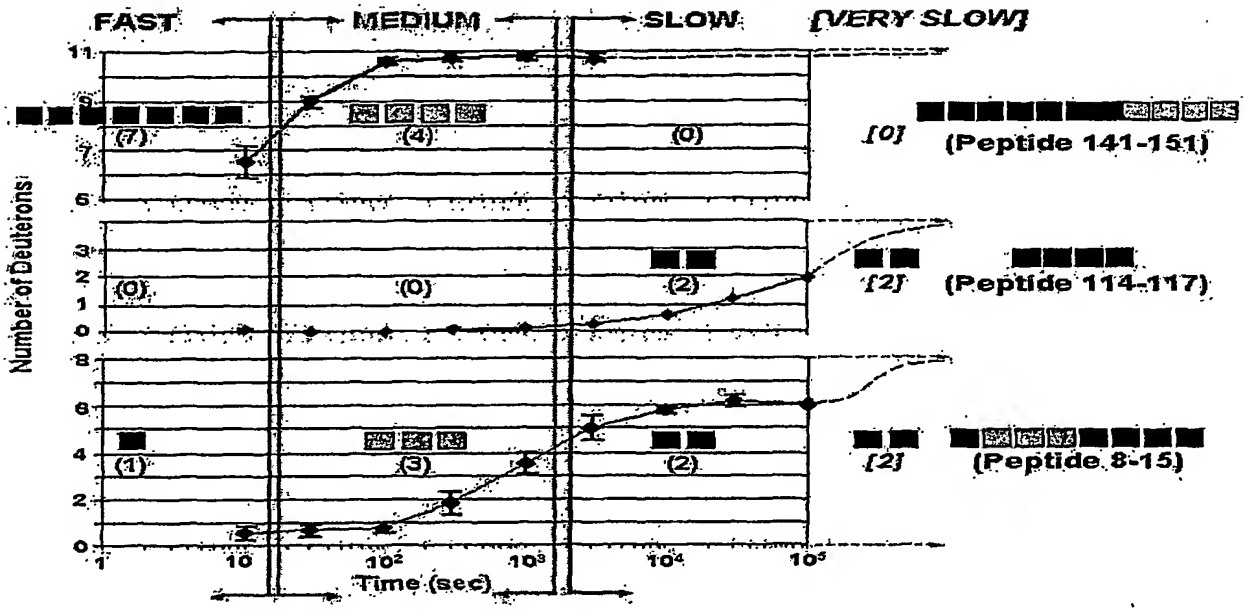
FAST
MEDIUM
SLOW
[VERY SLOW]
Number of Deuterons
Time (sec)
(Peptide 141-151)
(Peptide 114-117)
(Peptide 8-15)

Figure 10

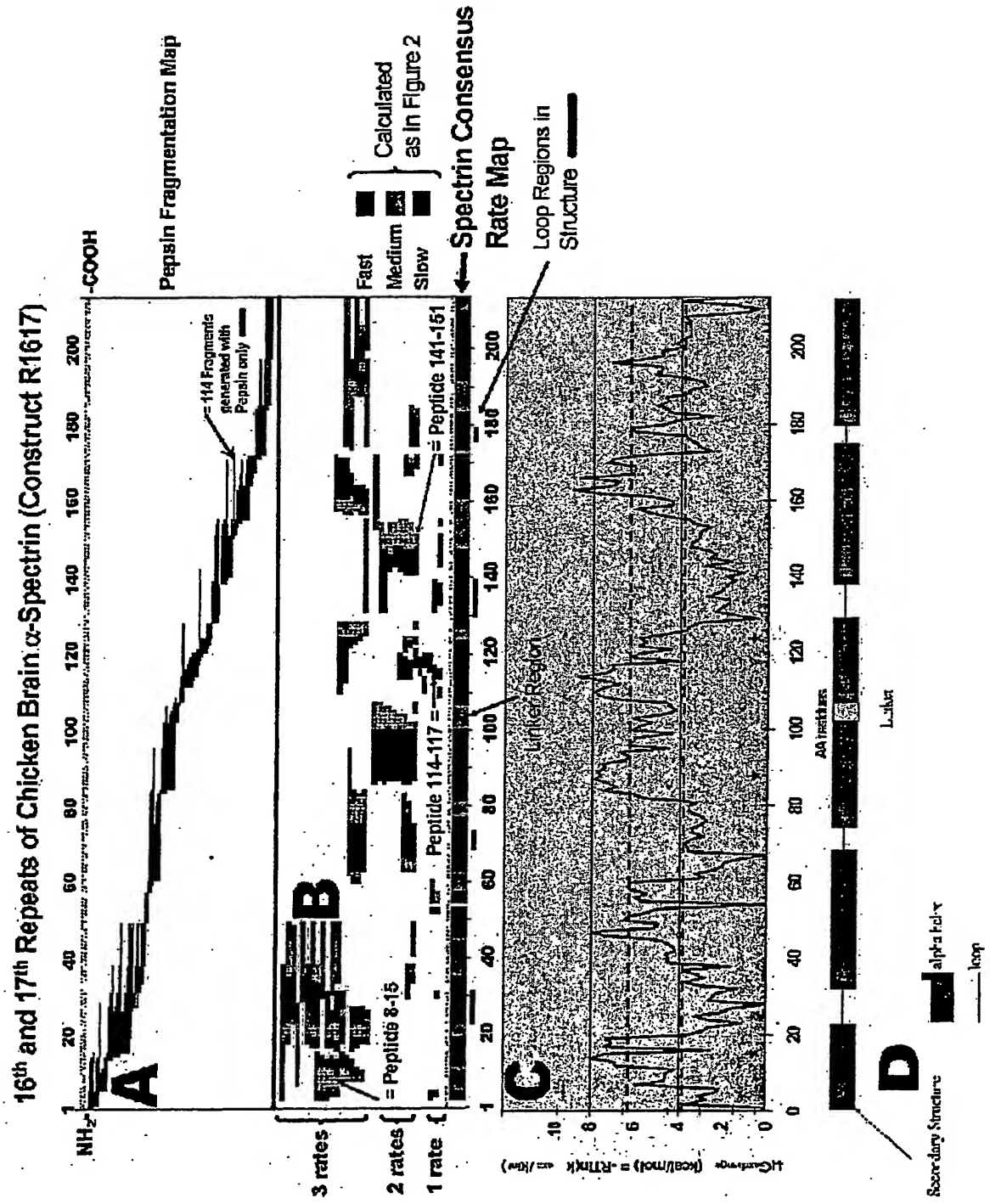
16th and 17th Repeats of Chicken Brain α-Spectrin (Construct R1617)
A
Pepsin Fragmentation Map
NH2
-COOH
= 114 Fragments generated with Pepsin only
B
Fast
Medium
Slow
Calculated as in Figure 2
Spectrin Consensus Rate Map
3 rates
2 rates
1 rate
= Peptide 8-15
= Peptide 114-117
= Peptide 141-151
Loop Regions in Structure
C
Linked Region
D
Secondary Structure
alpha helix
loop
Label

Figure 11

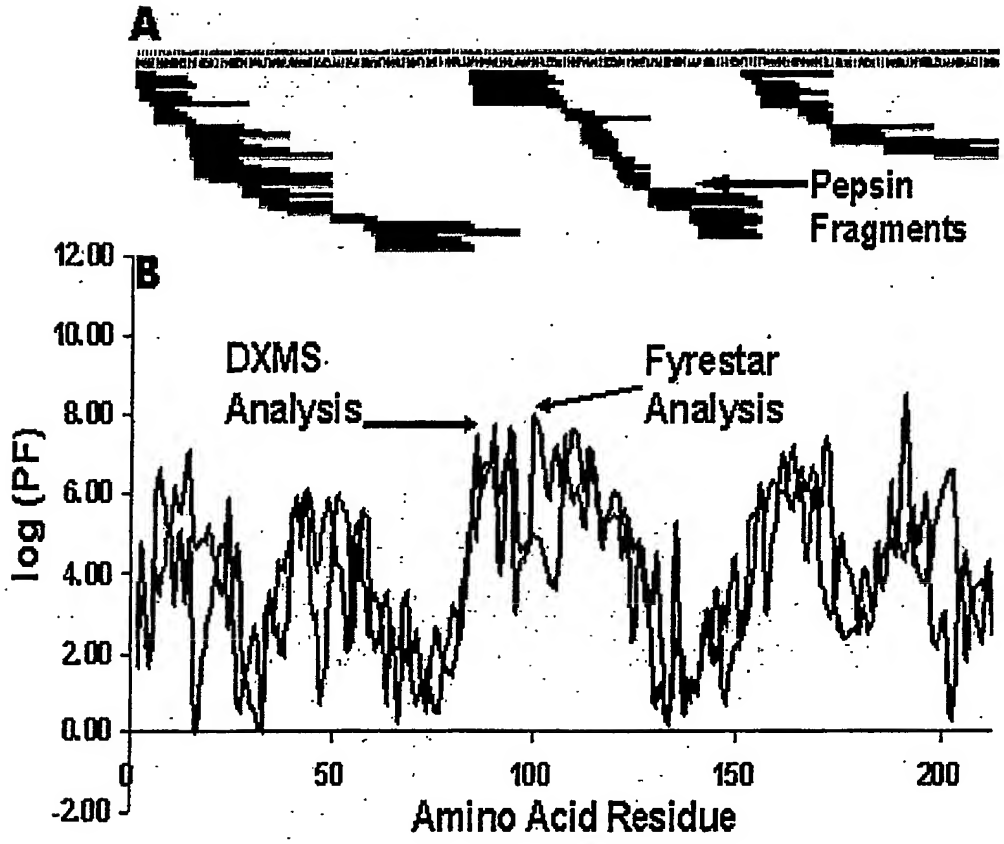
A
Pepsin
Fragments
B
DXMS
Analysis
Fyrestar
Analysis
log (PF)
12.00
10.00
8.00
6.00
4.00
2.00
0.00
-2.00
0
50
100
150
200
Amino Acid Residue

Figure 12

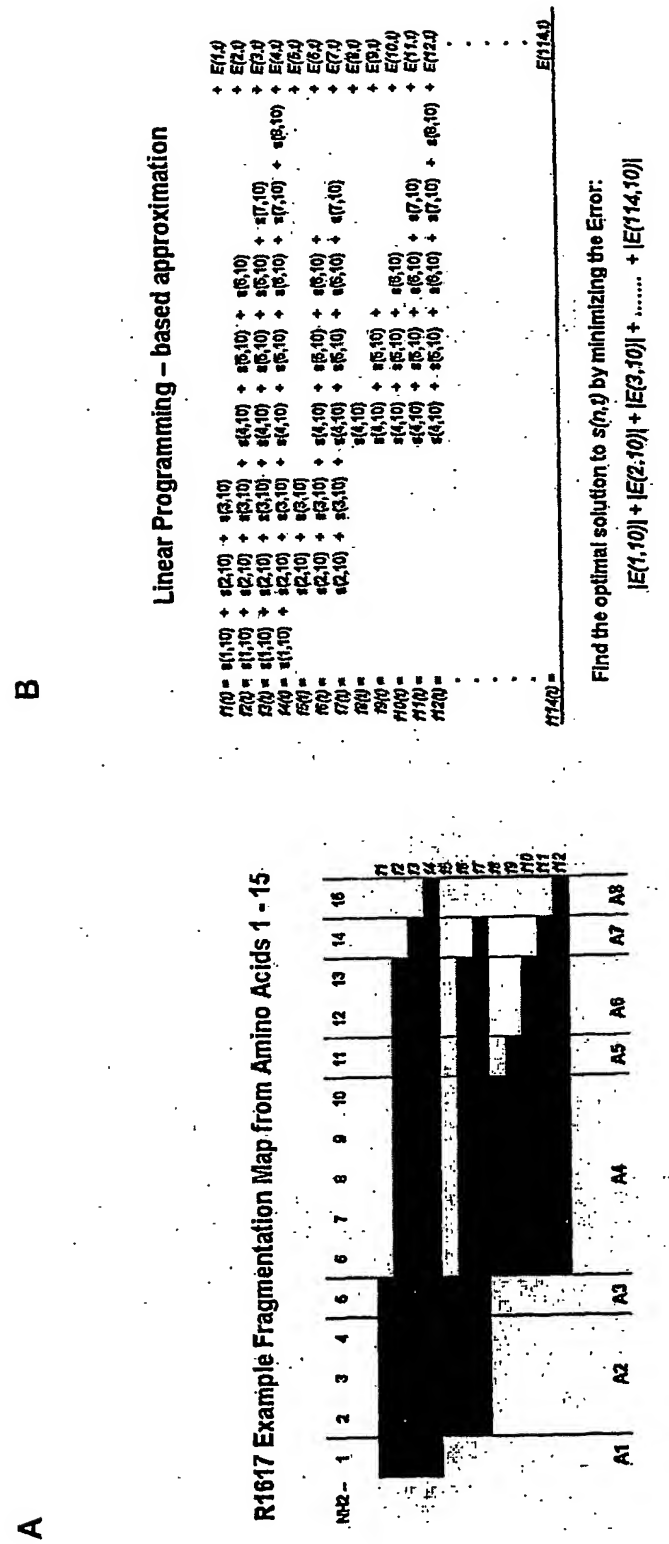
A
R1617 Example Fragmentation Map from Amino Acids 1 - 15
NH2 –
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16
A1 A2 A3 A4 A5 A6 A7 A8
B
Linear Programming – based approximation
Find the optimal solution to s(n,t) by minimizing the Error:
|E(1,10)| + |E(2,10)| + |E(3,10)| + ... + |E(114,10)|

Figure 13

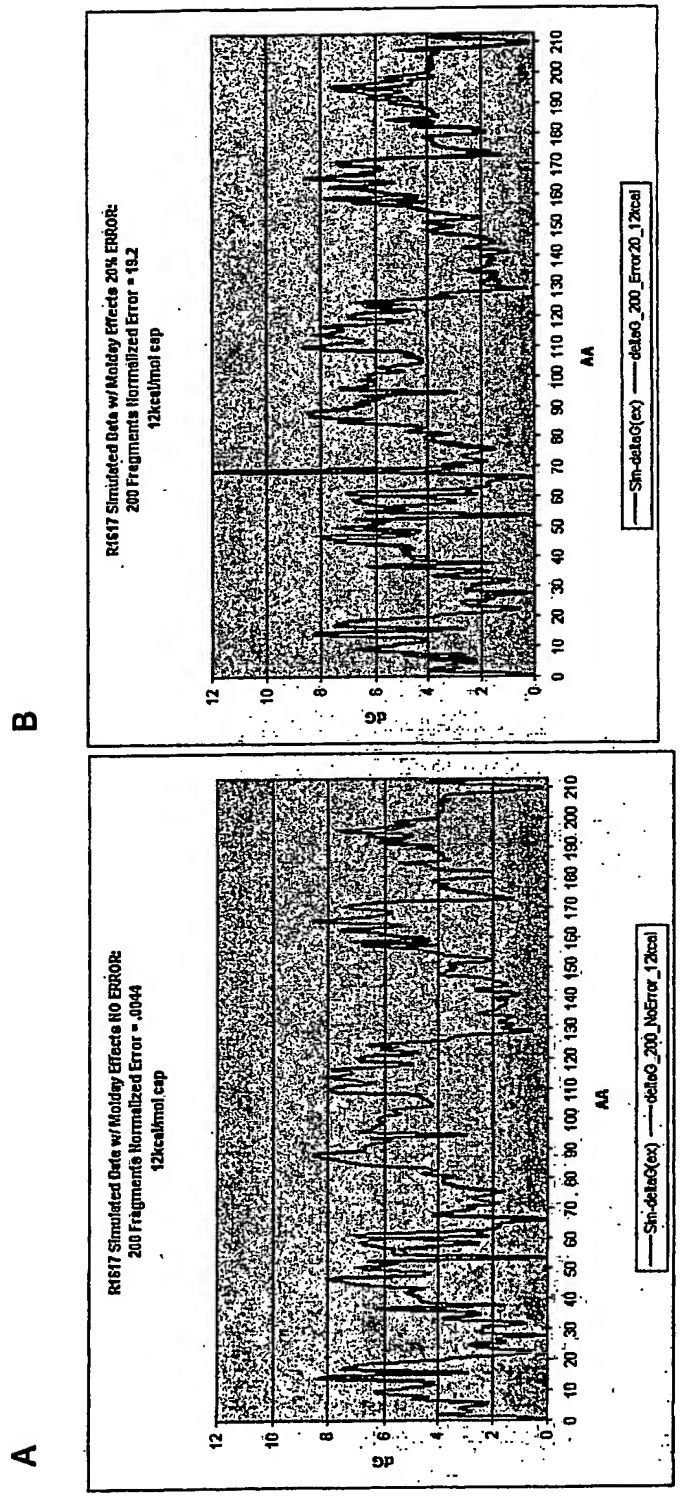
A
R1617 Simulated Data w/ Moldey Effects NO ERROR
200 Fragments Normalized Error = .0044
12kcal/mol cap
dG
AA
Sln-deltaG(ex)
deltaG_200_NoError_12kcal
B
R1617 Simulated Data w/ Moldey Effects 20% ERROR
200 Fragments Normalized Error = 19.2
12kcal/mol cap
dG
AA
Sln-deltaG(ex)
deltaG_200_Error20_12kcal

Figure 14

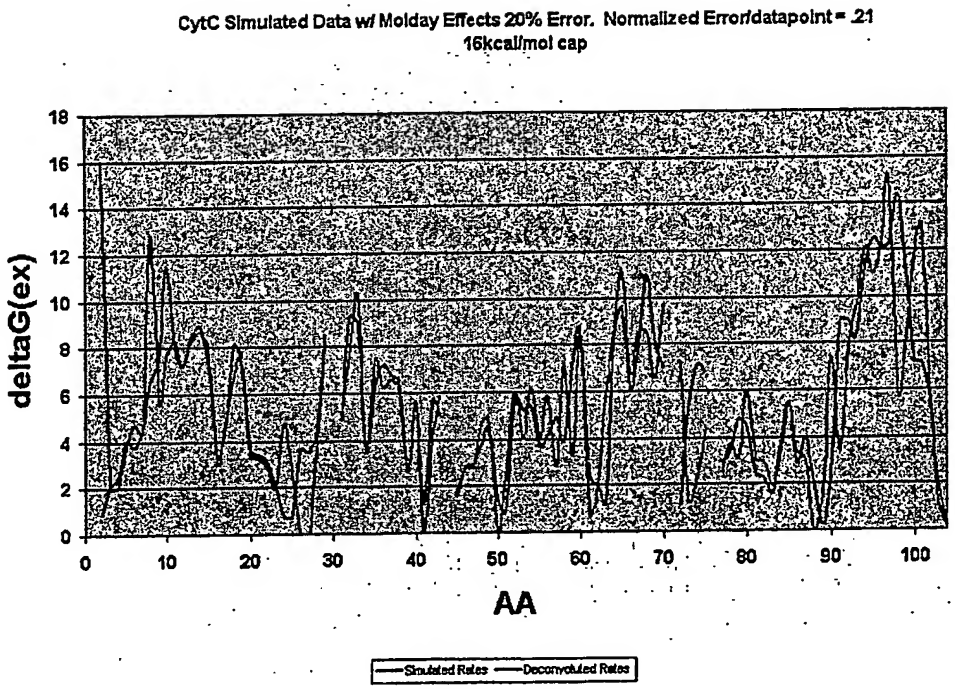
CytC Simulated Data w/ Molday Effects 20% Error. Normalized Error/datapoint = .21
16kcal/mol cap
deltaG(ex)
AA
Simulated Rates
Deconvoluted Rates

Figure 15

This Page is Inserted by IFW Indexing and Scanning Operations and is not part of the Official Record

BEST AVAILABLE IMAGES

Defective images within this document are accurate representations of the original documents submitted by the applicant.

Defects in the images include but are not limited to the items checked:

- ☐ BLACK BORDERS
- ☐ IMAGE CUT OFF AT TOP, BOTTOM OR SIDES
- ☑ FADED TEXT OR DRAWING
- ☑ BLURRED OR ILLEGIBLE TEXT OR DRAWING
- ☐ SKEWED/SLANTED IMAGES
- ☐ COLOR OR BLACK AND WHITE PHOTOGRAPHS
- ☐ GRAY SCALE DOCUMENTS
- ☐ LINES OR MARKS ON ORIGINAL DOCUMENT
- ☐ REFERENCE(S) OR EXHIBIT(S) SUBMITTED ARE POOR QUALITY
- ☐ OTHER: _____

IMAGES ARE BEST AVAILABLE COPY.
As rescanning these documents will not correct the image problems checked, please do not report these problems to the IFW Image Problem Mailbox.